Higher-order isospin-symmetry-breaking corrections to nuclear matrix elements of Fermi β decays

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Within the nuclear shell model, we derive the exact expression for the isospin-symmetry breaking correction to the nuclear matrix element of Fermi β decays. Based on a perturbation expansion in small quantities, such as the deviation of the overlap integral between proton and neutron radial wave functions from unity and of the transition density from its isospin-symmetry value, we demonstrate that δ_C can be obtained as a sum of six terms. These terms comprise two leading order (LO) terms, two next-to-leading order (NLO) terms, one next-to-next-to-leading order (NNLO) term, and one next-to-next-to-next-to-leading order (NNNLO) term. While the first two terms have been considered in a series of shell-model calculations [J. C. Hardy and I. S. Towner, Phys. Rev. C **102**, 045501 (2020), and references therein], the remaining four terms have been neglected. A numerical calculation has been carried out for 24 superallowed $0^+ \to 0^+$ transitions (18 isotriplets and six isoquintets) and three non-$0^+ \to 0^+$ transitions, across the p to pf shells. For most $0^+ \to 0^+$ transitions, the higher-order contribution is of the order 10^{-3}% or smaller, well below the typical theoretical errors quantified within the shell model with Woods-Saxon radial wave functions given in the reference cited above. However, for specific cases such as ^{70}Br and ^{74}Rb, where weakly bound effect dominates, it increases considerably, becoming comparable to or even exceeding the errors in the isospin mixing component of the LO terms. In the cases of ^{20}Mg and ^{48}Fe, as well as in non-$0^+ \to 0^+$ transitions, the higher-order contribution becomes more substantial. Notably, it reaches as large as -4.460% in ^{31}Cl and -2.027% in ^{32}Cl, due to the concurrent effect of the weakly bound and strong isospin mixing in their daughter nuclei. In contrast, for ^{26}P, the NLO terms, despite their substantial magnitude, effectively cancel each other out due to their opposite signs.

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I. INTRODUCTION

The standard-model description of Fermi β decay includes only the vector currents of the electroweak interaction. This important feature provides a very simple relationship between the vector-coupling constant, G_V, and the ft value with theoretical corrections of the order of a few percent being applied to account for radiative effects and for isospin-symmetry breaking between a parent and a daughter state (see a recent review [1] and references therein). It is customary to define a corrected $\mathcal{F}t$ value via

$$\mathcal{F}t = ft(1+\delta_R')(1-\delta_C+\delta_{NS}) = \frac{K}{|\mathcal{M}_F|^2 G_V^2 (1+\Delta_R^V)}, \quad (1)$$

where ft is the product of the statistical rate function (f) and the partial half-life (t) [2], K is a combination of fundamental constants [1], δ_C is the correction for the breaking of the isospin symmetry which is the main interest of the present study. The quantities Δ_R^V, δ_R', and δ_{NS} are the nucleus-independent, the (Z, Q_{EC})-dependent, and the nuclear-structure-dependent radiative corrections, respectively [1]. The Fermi matrix element in the isospin-symmetry limit is model-independent and can be expressed as

$$|\mathcal{M}_F|^2 = T(T+1) - T_{zi}T_{zf}, \quad (2)$$

where T is the isospin quantum number of the multiplet, and T_{zi} and T_{zf} are the isospin projection quantum numbers of the initial and final nucleus, respectively. For an isospin triplet ($T = 1$) we obtain $|\mathcal{M}_F|^2 = 2$ and hence $\mathcal{F}t$ should be a nucleus-independent quantity.

As was discovered first by Cabibbo [3], and generalized further by Kobayashi and Maskawa [4], the vector-coupling constant, G_V, governing a semileptonic weak process is different from the universal Fermi coupling constant, G_μ, responsible for a purely leptonic weak decay [1,5]. The reason is that quarks participating in the weak interaction are superposition of the quark mass eigenstates. This leads to appearance of the quark mixing matrix, or Cabbibo-Kobayashi-Maskawa (CKM) matrix, in the charge-changing weak interaction Lagrangian. For a nucleon weak decay,

$$G_V = G_\mu |V_{ud}|, \quad (3)$$

where V_{ud} is the upper-left element of the CKM matrix.

Therefore, precise determinations of ft values together with theoretical corrections provide crucial information on the

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electroweak force and put constraints on physics beyond the standard model. For example, the constancy of $\mathcal{F}t$ values for all $J^\pi = 0^+, T = 1 \to J^\pi = 0^+, T = 1$ decays would serve as a direct test of the conserved vector current (CVC) hypothesis. The current average $\mathcal{F}t$ value for the 15 best-known superallowed transitions of isotriplets over a mass region of $10 \leqslant A \leqslant 74$ is [1]

$$\overline{\mathcal{F}t} = 3072.24 \pm 1.85 \text{ sec} \tag{4}$$

with $\chi^2/\nu = 0.47$.

In addition, if CVC is confirmed, $|V_{ud}|$ can be extracted with a great precision from $\overline{\mathcal{F}t}$ via Eqs. (3) and (1), which is important for the unitarity tests of the CKM matrix. Those tests would put stringent limits on possible physics beyond the standard model, such as the presence of scalar terms or right-handed currents. Further details and the current status of the domain can be found in Ref. [1].

Although the δ_C correction is small, it is significant, and its associated theoretical errors, at present, dominate the uncertainty of $|V_{ud}|$ because of the very high precision reached on the experimental side and in the calculation of radiative corrections [1]. Within the shell-model approach [6–8], δ_C is usually separated in two components, namely,

$$\delta_C \approx \delta_{C1} + \delta_{C2}, \tag{5}$$

where the first term on the right-hand side (r.h.s.) appears due to isospin-symmetry breaking effects in the configuration mixing induced by isospin-nonconserving forces in an effective shell-model Hamiltonian, whereas the second term accounts for a mismatch between neutron and proton single-particle radial wave functions.

Calculations based on Eq. (5) have provided the best set of δ_C values in eliminating the considerable scatters present within the uncorrected ft values and, at the same time, excellently supported the top-row unitarity of the CKM matrix (see for example Refs. [1,9]). However, we recall that expression (5) is only a lowest order approximation and its validity should be tested numerically for a wide variety of nuclei. The splitting of the correction into two terms was criticized by some authors, e.g., [10]. At the same time, direct calculation of the realistic Fermi matrix element using isospin-nonconserving shell-model Hamiltonian and realistic single-particle wave functions is very slowly converging. In our previous study we were limited to lighter nuclei [11]. It is the purpose of the present study to derive a suitable formalism for missing higher order terms and to estimate their values from a numerical calculation in the framework of the shell model with Woods-Saxon radial wave functions.

The paper is structured as follows. In Sec. II we present our theoretical formalism based on the shell model. Namely, starting from the basic definition of the Fermi β decay matrix element within the closure approximation, we derive the isospin-symmetry-breaking corrections, including the leading order (LO) and the higher order terms, and we discuss their properties. In the last part of this section, we generalize this idea and derive expressions for corrections within the parentage expansion formalism. In Sec. III, we present numerical calculations of the higher order terms and discuss their possible impact on the Fermi matrix element, as well as their relevance for the tests of the standard model. Conclusions and perspectives are given in Sec. IV.

II. GENERAL SHELL-MODEL FORMALISM

A. Closure approximation

As a first step for deriving the exact shell-model expression of δ_C, we write the nuclear matrix element for a Fermi transition from an initial state $|i\rangle$ to a final state $|f\rangle$ in the angular momentum coupled form, namely,

$$M_F^{\pm} = \sum_{k_a k_b} \langle k_a \tau_a \| \tau_\pm \| k_b \tau_b \rangle \text{OBTD}(k_a \tau_a k_b \tau_b i f \lambda), \tag{6}$$

where $|k_a\tau_a\rangle \in |f\rangle$ and $|k_b\tau_b\rangle \in |i\rangle$ with $k_{a/b}$ standing for the set of spherical quantum number (nlj) of state a/b and $\tau_{a/b}$ for the isospin projection quantum number (we use the isospin convention of $\tau_p = -\frac{1}{2}$ for protons and $\tau_n = \frac{1}{2}$ for neutrons). The $\pm$ sign corresponds to the nuclear $\beta^\pm$ decay and $\tau_\pm$ is the isospin raising (upper sign)/lowering (lower sign) operator. The one-body transition density (OBTD) is defined as

$$\text{OBTD}(k_a \tau_a k_b \tau_b i f \lambda) = \frac{\langle f \| \left[a^\dagger_{k_b \tau_b} \otimes \tilde{a}_{k_b \tau_b} \right]^\lambda \| i \rangle}{\sqrt{2\lambda + 1}}, \tag{7}$$

where $\lambda = 0(1)$ for Fermi (Gamow-Teller) β decay. The double bars in the reduced matrix elements in Eqs. (6) and (7) denote a reduction in angular momentum space.

The reduced single-particle matrix element in Eq. (6) can be written in a close form as follows:

$$\langle k_a \tau_a \| \tau_\pm \| k_b \tau_b \rangle = \theta_F(l_a l_b j_a j_b) \Omega^{\tau_a \tau_b}_{k_a k_b} \xi_{\tau_a \tau_b}, \tag{8}$$

where the first factor, $\theta_F(l_a l_b j_a j_b)$, depends on the orbital and total angular momenta of the single-particle states involved, and therefore specifies information on the transition's selection rule. For a Fermi operator, acting between the states of the same isospin multiplet (*isobaric analog states*), the function $\theta_F(l_a l_b j_a j_b)$ has a very simple expression

$$\theta_F(l_a l_b j_a j_b) = \sqrt{(2j_a + 1)} \delta_{l_a l_b} \delta_{j_a j_b}. \tag{9}$$

The second factor on the r.h.s. of Eq. (8), $\Omega^{\tau_a \tau_b}_{k_a k_b}$, is the overlap integral of single-particle radial wave functions:

$$\Omega^{\tau_a \tau_b}_{k_a k_b} = \int_0^\infty R^{\tau_a}_{k_a}(r) R^{\tau_a}_{k_b}(r) r^2 dr < 1. \tag{10}$$

Note that if one uses harmonic oscillator functions which are isospin-invariant as employed in the conventional shell model, $\Omega^{\tau_a \tau_b}_{k_a k_b}$ reduces to the normalization integral. However, with realistic single-particle wave functions, such as the eigenfunctions of Woods-Saxon or Hartree-Fock potentials with Coulomb and nuclear isovector terms included, the integral $\Omega^{\tau_a \tau_b}_{k_a k_b}$ slightly deviates from unity. Furthermore, the inclusion of an isospin-nonconserving term in the mean-field potential leads to a nodal mixing in the eigenfunctions, and hence transitions between orbitals with different numbers of nodes are not strictly forbidden [12,13]. In general, this effect cannot be taken into account in a straightforward manner, because of the requirement of a huge model space.

The isospin component, $\xi_{\tau_a \tau_b}$, of Eq. (8) is given by

$$\xi_{\tau_a \tau_b} = \langle \tau_a | \tau_\pm | \tau_b \rangle = \begin{cases} 1 & \text{for } \tau_b = \tau_a \mp 1, \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

Within the framework of the shell model with a realistic basis, isospin-symmetry breaking can impact the nuclear matrix element of the Fermi operator in two different ways: i) it creates differences in the structure of the initial and final states due to isospin mixing induced by isospin-nonconserving components of the effective shell-model Hamiltonian (this leads to the deviation of one-body transition densities from their isospin-symmetry-limit values), and ii) it causes deviation of the overlap integrals (10) from unity due to Coulomb and nuclear isovector terms present in a realistic mean-field potential. Both effects lead to a reduction in absolute value of the Fermi matrix element [6].

Therefore, it is natural to rearrange the $M_F^{\pm}$ expression as

$$\begin{aligned} M_F^{\pm} = &\sum_{k_a k_b} \theta_F(l_a l_b j_a j_b)\xi_{\tau_a\tau_b}\mathrm{OBTD}^T(k_a\tau_a k_b\tau_b i f\lambda) \\ &- \sum_{k_a k_b} \theta_F(l_a l_b j_a j_b)\Lambda^{\tau_a\tau_b}_{k_a k_b}\xi_{\tau_a\tau_b}\mathrm{OBTD}^T(k_a\tau_a k_b\tau_b i f\lambda) \\ &- \sum_{k_a k_b} \theta_F(l_a l_b j_a j_b)\xi_{\tau_a\tau_b} D(k_a\tau_a k_b\tau_b i f\lambda) \\ &+ \sum_{k_a k_b} \theta_F(l_a l_b j_a j_b)\Lambda^{\tau_a\tau_b}_{k_a k_b}\xi_{\tau_a\tau_b} D(k_a\tau_a k_b\tau_b i f\lambda), \end{aligned} \tag{12}$$

where $\mathrm{OBTD}^T(k_a\tau_a k_b\tau_b i f\lambda)$ stands for the isospin-symmetry limit of the one-body transition density and $D(k_a\tau_a k_b\tau_b i f\lambda)$ for its deviation from the corresponding isospin-nonconserving value:

$$\begin{aligned} D(k_a\tau_a k_b\tau_b i f\lambda) = &\,\mathrm{OBTD}^T(k_a\tau_a k_b\tau_b i f\lambda) \\ &- \mathrm{OBTD}(k_a\tau_a k_b\tau_b i f\lambda). \end{aligned} \tag{13}$$

The quantity $\Lambda^{\tau_a\tau_b}_{k_a k_b}$ denotes the deviation from unity of the overlap integral, i.e.,

$$\Lambda^{\tau_a\tau_b}_{k_a k_b} = 1 - \Omega^{\tau_a\tau_b}_{k_a k_b}. \tag{14}$$

We remark that $\Lambda^{\tau_a\tau_b}_{k_a k_b}$ is always positive, while $D(k_a k_b i f\lambda)$ can be either positive or negative. In what follows we consider transitions between states for which isospin-symmetry is only weakly broken. In this case, $\Lambda^{\tau_a\tau_b}_{k_a k_b}$ and $D(k_a k_b i f\lambda)$ are sufficiently small quantities, so they can serve as perturbation parameters.

The first term on the r.h.s. of Eq. (12) corresponds to the Fermi matrix element in the isospin-symmetry limit, $\mathcal{M}_F^{\pm}$. We can therefore use it to factorize Eq. (12) as

$$\begin{aligned} M_F^{\pm} = \mathcal{M}_F^{\pm}\Bigg[1 &- \frac{1}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\Lambda^{\tau_a\tau_b}_{k_a k_b}\xi_{\tau_a\tau_b} \\ &\times \mathrm{OBTD}^T(k_a\tau_a k_b\tau_b i f\lambda) \\ &- \frac{1}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\xi_{\tau_a\tau_b} D(k_a\tau_a k_b\tau_b i f\lambda) \\ &+ \frac{1}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\Lambda^{\tau_a\tau_b}_{k_a k_b}\xi_{\tau_a\tau_b} D(k_a\tau_a k_b\tau_b i f\lambda)\Bigg]. \end{aligned} \tag{15}$$

The last three terms on the r.h.s. of Eq. (15) appear due to isospin-nonconservation. If isospin symmetry is preserved, those terms vanish and, hence, $M_F^{\pm} = \mathcal{M}_F^{\pm}$.

At the next step, we square both sides of Eq. (15) and rearrange the result in the following form:

$$|M_F^{\pm}|^2 = |\mathcal{M}_F^{\pm}|^2(1 - \delta_C), \tag{16}$$

where the total isospin-symmetry-breaking correction, δ_C, represents a sum of six terms:

$$\delta_C = \overline{\delta}_{C1} + \overline{\delta}_{C2} + \overline{\delta}_{C3} + \overline{\delta}_{C4} + \overline{\delta}_{C5} + \overline{\delta}_{C6}. \tag{17}$$

Here, the bar indicates that the correction terms are evaluated within the closure approximation. A more extended treatment is present in Sec. II B.

The first and second terms on the r.h.s. of Eq. (17) are the two usual LO terms. It is interesting to note that, at this lowest order approximation, the isospin mixing and the radial mismatch effects can be accounted for as two separate correction terms. The isospin-mixing correction corresponds to $\overline{\delta}_{C1}$. This correction term is calculated using an isospin-nonconserving effective shell-model Hamiltonian and the harmonic oscillator basis, such as

$$\begin{aligned} \overline{\delta}_{C1} &= \frac{2}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\xi_{\tau_a\tau_b} D(k_a\tau_a k_b\tau_b i f\lambda), \\ &= 2 - \frac{2}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\xi_{\tau_a\tau_b} \\ &\quad\times \mathrm{OBTD}(k_a\tau_a k_b\tau_b i f\lambda). \end{aligned} \tag{18}$$

The radial mismatch correction corresponds to $\overline{\delta}_{C2}$. This correction term is calculated using an isoscalar effective shell-model Hamiltonian and realistic radial wave functions, namely,

$$\begin{aligned} \overline{\delta}_{C2} &= \frac{2}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\Lambda^{\tau_a\tau_b}_{k_a k_b}\xi_{\tau_a\tau_b} \\ &\quad\times \mathrm{OBTD}^T(k_a\tau_a k_b\tau_b i f\lambda), \\ &= 2 - \frac{2}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\Omega^{\tau_a\tau_b}_{k_a k_b}\xi_{\tau_a\tau_b} \\ &\quad\times \mathrm{OBTD}^T(k_a\tau_a k_b\tau_b i f\lambda). \end{aligned} \tag{19}$$

The third and the fourth terms on the r.h.s. of Eq. (17) are the next-to-leading order (NLO) terms. The former depends on both $\Lambda^{\tau_a\tau_b}_{k_a k_b}$ and $D(k_a\tau_a k_b\tau_b i f\lambda)$, therefore it must be evaluated using both an isospin non-conserving Hamiltonian and realistic radial wave functions. It can be expressed as

$$\begin{aligned} \overline{\delta}_{C3} &= -\frac{2}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\Lambda^{\tau_a\tau_b}_{k_a k_b}\xi_{\tau_a\tau_b} D(k_a\tau_a k_b\tau_b i f\lambda), \\ &= -\overline{\delta}_{C2} + \frac{2}{\mathcal{M}_F^{\pm}}\sum_{k_a k_b}\theta_F(l_a l_b j_a j_b)\Lambda^{\tau_a\tau_b}_{k_a k_b}\xi_{\tau_a\tau_b} \\ &\quad\times \mathrm{OBTD}(k_a\tau_a k_b\tau_b i f\lambda). \end{aligned} \tag{20}$$

In contrast, the latter is simply a function of the two LO terms, which can be written as

$$\bar{\delta}_{C4} = -\frac{(\bar{\delta}_{C1} + \bar{\delta}_{C2})^2}{4}. \tag{21}$$

The fifth and the sixth terms on the r.h.s. of Eq. (17) are the next-to-next-to-leading order (NNLO) and next-to-next-to-next-to-leading order (NNNLO) terms, respectively. $\bar{\delta}_{C5}$ is determined by the two NLO terms,

$$\bar{\delta}_{C5} = -\frac{(\bar{\delta}_{C1} + \bar{\delta}_{C2})\bar{\delta}_{C3}}{2} = -\bar{\delta}_{C3}\sqrt{|\bar{\delta}_{C4}|}, \tag{22}$$

while $\bar{\delta}_{C6}$ is determined only by $\bar{\delta}_{C3}$ as

$$\bar{\delta}_{C6} = -\frac{(\bar{\delta}_{C3})^2}{4}. \tag{23}$$

Apparently, one only needs to perform shell-model calculations for the first three terms of Eq. (17) because the other three terms are just combinations of them. It can be also noticed that the LO terms are generally positive as can be seen from the previous calculations [6,7], $\bar{\delta}_{C4}$ and $\bar{\delta}_{C6}$ are obviously negative, $\bar{\delta}_{C3}$ can be negative or positive, while the sign of $\bar{\delta}_{C5}$ is opposite to the sign of $\bar{\delta}_{C3}$.

B. Parentage expansion formalism

The proton and neutron single-particle wave functions used for the evaluation of the overlap integrals depend on the type and parametrization of the realistic single-particle potential. For example, Towner and Hardy [6] worked mainly with a phenomenological Woods-Saxon potential, whereas Ormand and Brown [8] employed a local equivalent potential based on a self-consistent Hartree-Fock calculation with an effective zero-range Skyrme interaction (see also a recent study in the latter approach in Ref. [14]). In both cases, the chosen potential was thoroughly readjusted so that the energy eigenvalues would match the experimental separation energies. This procedure ensures the robustness of radial wave functions in the asymptotic region, as is clear from the following equation:

$$R(r) \to \exp\left(-\frac{\sqrt{2m|\epsilon|}r}{\hbar}\right)$$

with ϵ and m denoting the single-particle energy and the nucleon mass, respectively.

In order to specify separation energies needed to constraint the potential depth we insert a complete set of states $|\pi\rangle$ of the $(A-1)$-nucleon system into the one-body transition densities in Eq. (7) between the creation and annihilation operators. As a result, δ_{C2} takes the form

$$\delta_{C2} = \frac{2}{\mathcal{M}_F^{\pm}} \sum_{k_a k_b \pi} \theta_F(l_a l_b j_a j_b) \Lambda_{k_a k_b}^{\tau_a \tau_b \pi} \xi_{\tau_a \tau_b} \Theta(j_a j_b J_i J_f J_\pi \lambda) \times A^T(f; \pi k_a \tau_a) A^T(i; \pi k_b \tau_b), \tag{24}$$

where $A^T(f;\pi k_a\tau_a)$ and $A^T(i;\pi k_b\tau_b)$ stand for the spectroscopic amplitudes obtained from an isoscalar effective shell-model Hamiltonian. They are defined as

$$A^T(f;\pi k_a\tau_a) = \frac{(f\|a^\dagger_{k_a\tau_a}\|\pi)}{\sqrt{2J_f+1}} \tag{25}$$

and

$$A^T(i;\pi k_b\tau_b) = \frac{(i\|a^\dagger_{k_b\tau_b}\|\pi)}{\sqrt{2J_i+1}}, \tag{26}$$

where J_i and J_f are angular momenta of the initial and final states, respectively.

Again, double bars in Eqs. (25) and (26) denote reduction in angular momentum space. It should be also noted that we use round brackets for an isospin-invariant many-particle state. $\Lambda_{k_a k_b}^{\tau_a\tau_b}$ in Eq. (24) contains an additional label π, indicating that it is evaluated with radial wave functions whose asymptotic form matches separation energies with respect to excited states of the $(A-1)$-nucleon system. More details can be found in Ref. [6].

The function $\Theta(j_a j_b J_i J_f J_\pi \lambda)$ appearing in Eq. (24) is given by

$$\Theta(j_a j_b J_i J_f J_\pi \lambda) = \sqrt{(2J_i+1)(2J_f+1)}(-1)^{J_f+J_\pi+j_a+\lambda} \times \begin{Bmatrix} J_i & J_f & \lambda \\ j_b & j_a & J_\pi \end{Bmatrix}, \tag{27}$$

where J_π is the angular momentum of the intermediate state $|\pi\rangle$.

In the same way, the expression of δ_{C3} is evaluated as

$$\delta_{C3} = -\delta_{C2} + \frac{2}{\mathcal{M}_F^{\pm}} \sum_{k_a k_b \pi} \theta_F(l_a l_b j_a j_b) \Lambda_{k_a k_b}^{\tau_a \tau_b \pi} \xi_{\tau_a \tau_b} \times \Theta(j_a j_b J_i J_f J_\pi \lambda) A(f;\pi k_a \tau_a) A(i;\pi k_b \tau_b). \tag{28}$$

It can be remarked here that the structure of the second term on the r.h.s. of Eq. (28) looks very similar to that of δ_{C2}, except that $A^T(f;\pi k_a\tau_a)$ and $A^T(i;\pi k_b\tau_b)$ are replaced with the spectroscopic amplitudes calculated using an isospin non-conserving shell-model Hamiltonian (without superscript T). Furthermore, δ_{C3} will be negative if this term is smaller than δ_{C2} and positive in the opposite case.

In contrast, the isospin-mixing correction [the first term on the r.h.s. of Eq. (17)] is not affected by this expansion because it does not depend on radial wave functions. Therefore, we can write

$$\delta_{C1} = \bar{\delta}_{C1}. \tag{29}$$

All the other correction terms must be re-evaluated, taking into account the parentage expansion. In particular, δ_{C4} becomes

$$\delta_{C4} = -\frac{(\delta_{C1} + \delta_{C2})^2}{4}, \tag{30}$$

the new expression for δ_{C5} reads

$$\delta_{C5} = -\frac{(\delta_{C1} + \delta_{C2})\delta_{C3}}{2}, \tag{31}$$

and similarly for δ_{C6} we have

$$\delta_{C6} = -\frac{(\delta_{C3})^2}{4}. \tag{32}$$

We notice that calculations in the full parentage expansion formalism consume much more computational resources than calculations in the closure approximation. In general, 100 intermediate states of each spin and parity must be included, otherwise the corrections would not converge. The numerical aspects of the calculation of δ_{C2} for the superallowed Fermi transitions of isotriplets in the *sd* shell have been discussed in Ref. [7].

III. NUMERICAL CALCULATION OF THE HIGHER ORDER TERMS

Within the shell-model formalism discussed in the previous section, we have carried out a numerical calculation of the higher order terms for three distinct types of Fermi transitions, including

(i) Superallowed $0^+ \to 0^+$ transitions within isotriplets: ^{10}C, ^{14}O, ^{18}Ne, ^{22}Mg, ^{26m}Al, ^{26}Si, ^{30}S, ^{34}Cl, ^{34}Ar, ^{42}Ti, ^{46}V, ^{46}Cr, ^{50}Mn, ^{50}Fe, ^{54}Co, ^{54}Ni, ^{70}Br, and ^{74}Rb,
(ii) Superallowed $0^+ \to 0^+$ transitions within isoquintets: ^{20}Mg, ^{24}Si, ^{28}S, ^{32}Ar, ^{44}Cr, and ^{48}Fe, and
(iii) Non-$0^+ \to 0^+$ transitions, including those from the first 3^+, $T = 2$ state in ^{26}P, the first 1^+, $T = 1$ state in ^{32}Cl, and the first $\frac{3}{2}^+$, $T = \frac{3}{2}$ state in ^{31}Cl, where a strong isospin mixing in their final states has been observed [15–18].

We selected the Cohen-Kurath interaction [19] for nuclei with a mass between 10 and 14. For the next heavier nuclei up to $A = 25$, we chose the McGrory-Wildenthal-Reehal interaction [20]. For nuclei in the range of $18 \leqslant A \leqslant 34$, we utilized the well-known universal *sd*-shell interaction of Wildenthal [21], and for those with $42 \leqslant A \leqslant 74$, we employed the GXPF1A interaction developed by Honma and collaborators [22]. The respective configuration spaces are the full p, $p_{\frac{1}{2}} sd_{\frac{5}{2}}$, sd, and pf shells. To make our calculation tractable for ^{70}Br, a truncation has been imposed to the pf shell. The isospin non-conserving counterpart of the above cited shell-model effective Hamiltonians is comprised of isovector single-particle energies, the two-body Coulomb force between protons, and phenomenological charge-dependent nucleon-nucleon potentials of nuclear origin. Details of the fitting procedure are described in Ref. [23]. Our large-scale diagonalizations have been performed using the NuShellX@msu [24] shell-model code.

It can be noticed that in most cases, our chosen model spaces are smaller than those used in the calculations by Towner and Hardy [6]. We are aware that these reduced model spaces might not produce all necessary configurations for the initial and final states of the decays under consideration. Nevertheless, they should be sufficient for our present study which aims at exploring a relative magnitude of various subleading terms of the isospin-symmetry breaking correction.

The overlap integrals were evaluated with eigenfunctions of a phenomenological Woods-Saxon potential with the parametrization of Bohr and Mottelson [25], supplemented by modifications as described in Ref. [7]. In particular, the potential depth has been readjusted case by case in order to reproduce experimental separation energies, while accounting for excitations of the intermediate $(A-1)$-nucleon system. In addition, the Woods-Saxon length parameter has been simultaneously readjusted to reproduce the measured value of the charge radius of the parent nuclei. Note that, for a given transition, we have kept the length parameter the same for the initial and final nuclei. More details on the parameter adjustment, including our formalism for the charge radius calculation can be found in Ref. [7].

For the reason of consistency, we did not use the existing values of δ_{C1} and δ_{C2}, but we have recalculated them on equal footing with δ_{C3}. For the same reason, we did not scale δ_{C1} with the energy separation between the analog and the nearest nonanalog states in daughter nuclei as suggested by Towner and Hardy [6]. Moreover, since we are interested only in the relative magnitude between various correction terms, it is not necessary to consider uncertainties from the use of several effective shell-model Hamiltonians and from the charge radius data, which can be quantified using the method described in Refs. [6,26,27].

Our results for all correction terms are listed in Table I. Although the theoretical analysis in the previous section supposes that δ_{C1} and δ_{C2} are of the same order of magnitude, the calculated δ_{C1} values are generally considerably smaller than δ_{C2}. It is clearly seen that, for most cases, our calculated values for the two LO terms differ significantly from those of Towner and Hardy [6], the reason is related to the difference in configuration spaces, effective Hamiltonians, the Woods-Saxon parametrization and the potential-adjustment procedure.

It is interesting to remark that the sign of δ_{C3} varies from transition to transition as expected from the theoretical inspection in the previous section. We obtained a negative δ_{C3} value for ^{14}O, ^{34}Cl, ^{34}Ar, ^{50}Mn, and heavier emitters of the superallowed $0^+ \to 0^+$ transitions of isotriplets, ^{48}Fe (isoquintet), ^{31}Cl and ^{32}Cl (non-$0^+ \to 0^+$); while a positive value for the others. The primary reason is the non-monotonic nature of the isospin-mixing effect on the transition densities, causing the deviation $D(k_a \tau_a k_b \tau_b i f \lambda)$ to vary in sign and magnitude depending on the nucleus and orbitals. The signs of the other correction terms can be determined as follows. According to our numerical results, the absolute value of δ_{C3} is, on average, one order of magnitude smaller than δ_{C1} and two orders of magnitude smaller than δ_{C2}. We also see that δ_{C4} is, on average, of the same order of magnitude as δ_{C3}, but its sign is always negative, allowing for potential cancellations between these NLO terms in certain cases. As an illustration, the individual NLO terms for ^{26}P have substantial magnitudes compared to the $0^+ \to 0^+$ transitions, but their opposite signs lead to a negligible net contribution. Meanwhile, δ_{C5} and δ_{C6} are generally negligible, except for the cases of ^{31}Cl and ^{32}Cl due to very strong isospin mixing in the respective final states.

It does not appear that the higher order terms would increase dramatically with mass number. Nevertheless, they are influenced by the magnitude of the LO terms. In general, δ_{C2} is very sensitive to the weakly bound effect, as evident in cases such as ^{48}Fe, ^{70}Br, and ^{74}Rb, as well as the non-$0^+ \to 0^+$ transitions. On the other hand, δ_{C1} can be substantial if the

TABLE I. Calculated values of various terms of the isospin-symmetry-breaking correction in percent unit. Here, LO, NLO, NNLO, and NNNLO are the abbreviations for leading order, next-to-leading order, next-to-next-leading order, and next-to-next-to-next-leading order, respectively.

	LO		NLO		NNLO	NNNLO	NLO+NNLO+NNNLO
Emitter	δ_{C1}	δ_{C2}	δ_{C3}	δ_{C4}	δ_{C5}	δ_{C6}	$\delta_{C3}+\delta_{C4}+\delta_{C5}+\delta_{C6}$
^{10}C[a]	0.03421939	0.18931000	0.00049200	−0.00012491	−0.00000055	−0.00000000	0.00036654
^{14}O[a]	0.01016209	0.28316400	−0.00234000	−0.00021510	0.00000343	−0.00000001	−0.00255168
^{18}Ne[a]	0.00796504	0.20549300	0.00377500	−0.00011391	−0.00000403	−0.00000004	0.00365702
^{22}Mg[a]	0.01987732	0.26357900	0.00073900	−0.00020087	−0.00000105	−0.00000000	0.00053708
^{26m}Al[a]	0.00793319	0.26326700	0.00021200	−0.00018387	−0.00000029	−0.00000000	0.00002784
^{26}Si[a]	0.03037112	0.36937000	0.00058500	−0.00039948	−0.00000117	−0.00000000	0.00018435
^{30}S[a]	0.05890865	0.68247200	0.00514100	−0.00137411	−0.00001906	−0.00000007	0.00374776
^{34}Cl[a]	0.04336312	0.61015300	−0.00112700	−0.00106771	0.00000368	−0.00000000	−0.00219103
^{34}Ar[a]	0.00913932	0.70812600	−0.00055800	−0.00128617	0.00000200	−0.00000000	−0.00184217
^{42}Ti[a]	0.00577545	0.37658000	0.00068900	−0.00036549	−0.00000132	−0.00000000	0.00032219
^{46}V[a]	0.03266025	0.34878700	0.00029300	−0.00036376	−0.00000056	−0.00000000	−0.00007131
^{46}Cr[a]	0.02236702	0.44804100	0.00068200	−0.00055321	−0.00000160	−0.00000000	0.00012719
^{50}Mn[a]	0.04100000	0.46533600	−0.00076300	−0.00064094	0.00000193	−0.00000000	−0.00140201
^{50}Fe[a]	0.03724220	0.47617300	−0.00118200	−0.00065899	0.00000303	−0.00000000	−0.00183796
^{54}Co[a]	0.05146500	0.62774800	−0.00325900	−0.00115333	0.00001107	−0.00000003	−0.00440128
^{54}Ni[a]	0.08142300	0.67098900	−0.00164800	−0.00141531	0.00000620	−0.00000001	−0.00305712
^{70}Br[a]	0.46458999	1.39983500	−0.02944400	−0.00869020	0.00027448	−0.00000217	−0.03786189
^{74}Rb[a]	0.12627115	1.41762800	−0.07445100	−0.00595906	0.00057472	−0.00001386	−0.07984919
^{20}Mg[b]	0.13355259	0.70162193	0.06880904	−0.00174379	−0.00028734	−0.00001184	0.06676607
^{24}Si[b]	0.46641189	0.37229754	0.00623583	−0.00175858	−0.00002615	−0.00000010	0.00445099
^{28}S[b]	0.33713340	0.64352755	0.00402712	−0.00240424	−0.00001975	−0.00000004	0.00160309
^{32}Ar[b]	0.61163740	0.84563256	0.00065256	−0.00530909	−0.00000475	−0.00000000	−0.00466129
^{44}Cr[b]	0.03179293	0.33403410	0.00516561	−0.00033457	−0.00000945	−0.00000007	0.00482152
^{48}Fe[b]	0.93194417	1.03991361	−0.53696654	−0.00972056	0.00529411	−0.00072083	−0.54211382
^{26}P[c]	5.70963044	0.61244307	0.03669127	−0.09992153	−0.00115982	−0.00000336	−0.06439345
^{31}Cl[d]	30.50150797	2.69278055	−2.03182179	−2.75465198	0.33722439	−0.01032075	−4.45957012
^{32}Cl[e]	7.08669086	2.62265734	−1.87381996	−0.23567861	0.09096785	−0.00877800	−2.02730872

[a]Superallowed $0^+ \to 0^+$ Fermi β transition of isotriplets.
[b]Superallowed $0^+ \to 0^+$ Fermi β transition of isoquintets.
[c]$3^+ \to 3^+$ Fermi transition of isoquintet.
[d]$\frac{3}{2}^+ \to \frac{3}{2}^+$ Fermi transition of isoquartet.
[e]$1^+ \to 1^+$ Fermi transition of isotriplet.

initial or final states contain considerable isospin admixtures, as seen in the case of ^{48}Fe and the non-$0^+ \to 0^+$ transitions.

Therefore, the higher order terms could be significant if the LO terms are sufficiently large. In most cases of the superallowed $0^+ \to 0^+$ transitions within isotriplets, We obtain that the sum of all higher order terms (see the last column of Table I) is generally smaller than the uncertainties in the sum of the LO terms published in Ref. [6]. However, this behavior undergoes a dramatic change for ^{70}Br and ^{74}Rb, where the higher-order contribution becomes one to two orders of magnitude larger. This increase is primarily attributed to low proton separation energies and high occupancy in the $2p$ orbitals where centrifugal barrier is small. In these specific cases, the higher-order contribution is comparable to the uncertainties in δ_{C1} [6]. We emphasize that, in this theoretical approach, the precision of the dominant LO term, δ_{C2} is limited only by the charge radius data. For certain isoquintet cases such as ^{20}Mg and ^{48}Fe, as well as the non-$0^+ \to 0^+$ transitions, the higher-order contribution increases substantially because of the concurrent effect of the weakly bound and strong isospin mixing. In particular, it reaches −4.460% and −2.027% in ^{31}Cl and ^{32}Cl, respectively. Nevertheless, we cannot accurately quantify the theoretical uncertainties for these special transitions due to the lack of charge radius data for their emitter nuclei.

It is also interesting to emphasize that in the case of ^{32}Ar, both LO terms are also considerably larger than those in the cases of isotriplets, namely $\delta_{C1} \approx 0.612\%$ and $\delta_{C2} \approx 0.846\%$. However, the NLO terms do not increase accordingly, as observed in the other cases. This indicates a cancellation between the radial mismatch and isospin mixing occurring intrinsically within each individual NLO term.

IV. CONCLUSION AND PERSPECTIVE

We have developed a shell-model formalism for exact calculation of isospin-symmetry breaking correction to Fermi-transition matrix elements. Our special attention has been focused on the higher-order terms of this correction which were not considered in any of the previous shell-model

calculations. A numerical calculation has been carried out for 24 superallowed $0^+ \to 0^+$ transitions (18 isotriplets and six isoquintets) and three non-$0^+ \to 0^+$ transitions, across the p to pf shells. Our numerical results for the superallowed $0^+ \to 0^+$ transitions of isotriplets indicate that the higher-order contribution is generally smaller than the typical uncertainty in $\delta_{C1} + \delta_{C2}$ published in Ref. [1]. This supports earlier calculations that neglected these higher-order effects. However, while generally insignificant, the higher-order contribution increases by one to two orders of magnitude, becoming comparable with the uncertainties in δ_{C1} [1] for the two heaviest $N = Z$ emitters in the upper pf shell, namely ^{70}Br and ^{74}Rb, where the weakly bound effect dominates. A greater higher-order contribution is observed for certain superallowed $0^+ \to 0^+$ transitions of isoquintets, such as ^{20}Mg and ^{48}Fe, as well as for the three Fermi non-$0^+ \to 0^+$ transitions. In these nuclei, both the weakly bound effect and strong isospin mixing are simultaneously prominent.

Generally, the magnitude of higher-order terms would increase with increasing magnitude of the perturbation parameters (i.e., deviation of the overlap integrals from unity or the deviation of the one-body transition densities from their isospin-symmetry-limit values). Thus, higher-order terms, especially NLO terms, could be more substantial in the cases where the LO terms are extremely large, such as Fermi transitions of higher isospin multiplets, or when daughter nuclei exhibit strong isospin mixing, as seen in the three non-$0^+ \to 0^+$ transitions considered in this study. The theoretical formalism derived in this article can be easily generalized for other nuclear weak processes, particularly Gamow-Teller β decays whose mirror asymmetry is sensitive to the presence of the second class tensor current. Our analysis of the higher-order effects in Gamow-Teller β decays is under way and will be published separately.

For completeness, we recall that there are other possible sources of uncertainties of isospin-symmetry breaking correction, related to the certain ambiguity in the potential parametrization and to the choice of the shell-model Hamiltonians, lack of experimental data to constrain neutron wave function and other approximations of the theoretical formalism. The study of those effects, although beyond the scope of the present article, must be pursued to further reduce uncertainties of the theoretical modelization.

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